Ab initio Modeling of Superconducting Materials by Exploring Excited Electronic Configurations

William Tupa[1] and Dmitri Kilin[2]

[1]*Department of Physics, North Dakota State University, Fargo, ND 58108, United States*

[2]*Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND 58108, United States*

The high-pressure hydrogen sulfide material modified by methane maintains superconductive properties when at room temperature. This makes it a great candidate for industrial applications such as frictionless railway systems and power plants. We explore the electronic configuration features of this material relevant to superconductivity. Using constrained desity functional theory (DFT). Modification of electronic configurations includes changing the population of electronic states with certain values of spin projection, momentum, and energy.

We specifically focus on configurations of electrons with opposite spins and opposite values of momentum interacting via lattice, referred to as Cooper pairs. The goal of this ab initio research is to show that these pairs are available to form in the Hydrogen Sulfide material and can serve as the rational reason for superconductivity. The computed total energy of each electronic configuration is compared to the total energy of the reference neutral singlet configuration. This was done through VASP software for atomistic models of hydrogen sulfide with periodic boundary conditions. The results show that a configuration with a Cooper pair has the lowest energy among several explored configurations. The obtained ab initio results allow us to hypothesize that a combination of several configurations representing Cooper pairs would serve as a good start to model a collective condensate for a first principles evaluation of superconductivity. In the future, we plan to expand this consideration by quantitative evaluation of the nuclear reorganization induced by modification of electronic configuration.